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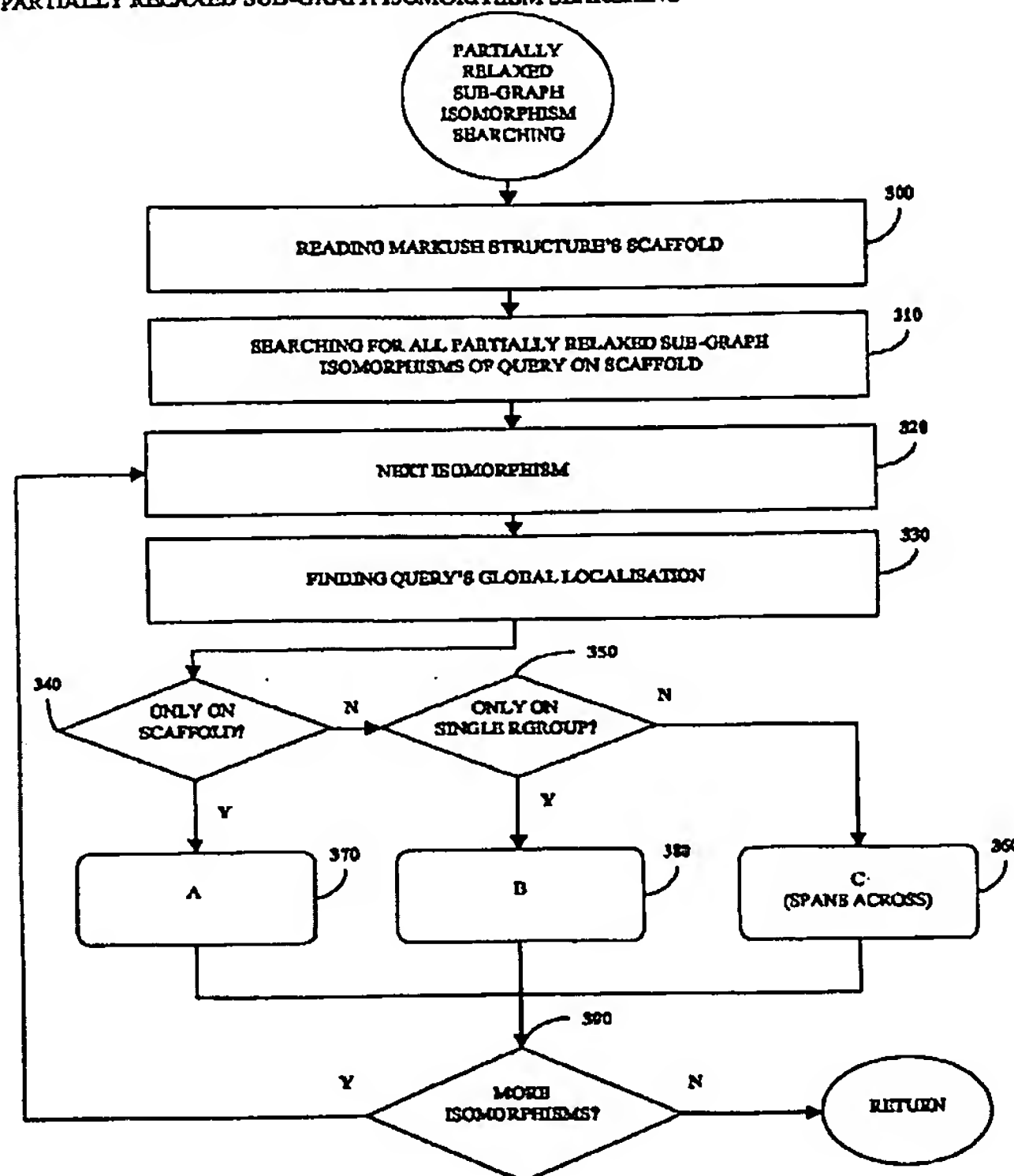
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(54) Title: **METHOD FOR FAST SUBSTRUCTURE SEARCHING IN NON-ENUMERATED CHEMICAL LIBRARIES**

SUBROUTINE:  
PARTIALLY RELAXED SUB-GRAPH ISOMORPHISM SEARCHING



(57) Abstract: The present invention relates generally to searching substructures in virtual combinatorial libraries. More precisely, it describes a method of operating a computer for searching substructures in large, non-enumerated virtual combinatorial libraries. Advantageously, the method can return matching products as non-enumerated substructures.